

# Dielectric confinement influenced screened Coulomb potential for a semiconductor quantum wire

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**Abstract.** A formalism of the Thomas-Fermi method has been applied for studying the screening effect due to quasi-one-dimensional electron gas in a semiconductor cylindrical quantum wire embedded in the barrier environment. With taking into account of strongly low dielectric properties of the barrier material, an applicability of the quantum wire effective interaction potential of the confined charge carriers has been revealed. Both screened quasi-one-dimensional interaction potential and effective screening length analytical expressions are derived in the first time. It is shown that in the long wavelength moderate limit dielectric confinement effect enhances strength of the screening potential depending on the both radius of the wire and effective screening length, whereas in the long wavelength strong limit the screening potential solely is determined by barrier environment dielectric properties.

## 1. Introduction

Wide interest to electron gas (EG) properties in quasi-one-dimensional (Q1D) semiconductor structures (quantum wires (QWR), nanorods, nano-whiskers or carbon nanotubes [1-4]) is initiated by application potential of these structures in high-speed electronic and optical devices [5]. A Q1D EG in these systems can be produced by intense optical illumination of a undoped QWR's or by modulating of the doping material [6]. An advanced selective doping makes it possible to spatially separate free carriers from the parent ionized impurities and to investigate charged Q1D carrier system rather than the neutral electron-hole plasma. As follows, a Q1D electron channel, confined in Q1D nanostructure (quantum confinement (QC)), can coexist with the confined coulomb centers (photo excited excitons, impurities) as in Q2D case [7] and screen Coulomb polarization fields between quasiparticles. In this sense, both the depth and wide scope of physics of the low-dimensional systems is mainly caused by strong quasiparticle correlations and weak screening of Coulomb interaction. Meanwhile the latter's strength and further enhancement are connected in the further lowering of the dimensionality of the nanostructure. In the 3D system Coulomb screened potential decays exponentially in real space and effectively becomes a short-range potential [8]. In a pure 2D structures Coulomb statically screened potential at the long-wavelength limit possess the 2D Coulomb law for the intermediate distances and power law spatial dependence for large distances, respectively [9, 10]. There is specific screening radius here and, in addition, screening parameter saturates both for the small temperature and large planar carrier density of the 2D EG. The Coulomb screening effect reducing takes place because free carriers can only screen Coulomb field between any two charges inside a low-dimensional system,



whereas a part of field extending outside the confinement region remains unscreened. It is assumed that this tendency should go on more strong by for the transition from quantum well (QW) to QWR.

The physical concept, that dielectric screening would be insufficient to reduce Coulomb repulsion between 1D (Q1D) confined charge carriers originates from the Kuper's work [11] and later this model reinvestigated in Ref.[12] by Davis. As a main result, the screened Coulomb potential expressions inside and outside the **conducting** 1D single-wire and coaxial cylinder are obtained in the Tomas-Fermi approximation (TFA). Subsequently, Lee and Spector [13] used random-phase approximation (RPA) to evaluate a screening potential of the charged impurity in **semiconducting** wire. Reyes et al. [14] derived both the dielectric function of 1D EG and asymptotic forms of the pure 1D screened Coulomb potential in semiconductor QWR by using 1D generalization of the TFA. Recently, Wang et al. [15] derived an analytical formula for the screened Q1D Coulomb potential in semiconductor Q1D nanostructures.

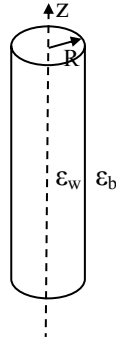
A realistic semiconductor QWR either can be freestanding or surrounded with a barrier environment. In this sense, for the Coulomb center-based structures, use of the low dielectric constant barrier environment of semiconductor QWR (lower than the semiconductor dielectric constant) is favorable, as it enhances the Coulomb interaction inside the QWR (dielectric confinement effect (DC)) [16-18]. The latter enhances both electronic and optical properties of the nanostructure and as a major result it becomes possible to implement "Coulomb interaction engineering" therein [16].

This tunability of the Coulomb interaction in the QWR due to the barrier environment dielectric properties enhances and modifies many body effects as well, in particular, dielectric screening effect of the Q1D EG. Most of the theoretical works in this area have been done by RPA framework to calculate the linear response of the QWR to an external charge in presence of the DC effect. Wendler and Grigoryan [19] by using a two-subband model an influence of the DC effect on the Q1D intra- and intersubband plasmon have studied. It has been shown that for a 1D long wave limit intrasubband plasmon possess a linear dispersion, is independent of the dielectric screening of the QWR and is wholly screened by surrounding barrier environment as in the Q2D intrasubband case [20]. Whereas by Aharonyan et al. in presence of the strong DC effect has been shown [21], that together with the previous result, which is consistent for the case of very small wave vectors only, there exists 1D moderate small wave vectors range in long wave limit as well, that collective plasmon frequencies are independent of the 1D wave vector and increase with decreasing of the QWR radius. Recently in Ref.[22] it is found that in the long-wavelength limit the dielectric screening and collective excitations of the Q1D EG are to be strongly influenced by barrier environment and exclusion of the DC effect in free-carrier screening results in an erroneous charged impurity scattering rate in QWR.

In the present paper we explore a general problem of determining the interaction potential of point charges pair confined within the semiconductor QWR embedded in the dielectric barrier environment and screened by Q1D EG. Our treatment sharply differs from that derived in Refs.13-15, where assumes that Q1D EG has homogeneous background having dielectric constant same as the barrier media.

## 2. CQWR model and TFA 3D screening potential

We are considering an infinitely long semiconductor cylindrical QWR (CQWR) of a radius  $R$  filled by the active material with the dielectric constant  $\epsilon_w$  and immersed in a dielectric barrier environment with the dielectric constant  $\epsilon_b$ . We have to argue, that the QWR infinite length concept allows us to discuss definite realistic semiconductor narrow samples, where one can used an adiabatic approximation of the Coulomb interaction. The latter replaces the three-dimensional potential of electrons and holes by a 1D Coulomb potential that describes their interaction along the QWR axis. In this sense, we are omitting a discussion in certain semiconductor quantum rod systems, where both the transverse and longitudinal dimensions have comparable sizes (for more details see for example [23]).



**Figure 1.** An infinitely long semiconductor cylindrical QWR (CQWR) of a radius  $R$  filled by the active material with the dielectric constant  $\epsilon_w$  and immersed in a dielectric barrier environment with the dielectric constant  $\epsilon_b$ .

Let us take in the cylindrical polar coordinates  $(\rho, \varphi, z)$ , where the  $z$  axis coincides with the CQWR axis. The sought interaction screened potential  $V_s(\rho, z) = e\Phi_s(\rho, z)$  of charges  $-e$  and  $e$  to be located at points  $(0, 0)$  and  $(\rho, z)$  respectively, is related to the induced charge density by generalized Poisson's equation

$$\begin{cases} \nabla^2 \Phi_s(r) = -\frac{4\pi e}{\epsilon_w} [\delta(r) - \Delta n^{ind}(r)], & \rho \leq R \\ \nabla^2 \Phi_s(r) = 0, & \rho > R \end{cases}, \quad (1)$$

where  $\Delta n^{ind}(\rho, z) = n^{ind}[\mu_0 + e\Phi_s(\rho, z)] - n^{ind}(\mu_0)$  is the variation of the density of EG,  $\mu_0$  is the chemical potential in the absence of the external perturbing field. Due to the cylindrical and reflection symmetry of the discussed problem Eq.(1) becomes independent of the angular coordinate  $\varphi$ .

In the equation system (1) we impose a constraint on the free electrons: the uniform local number density of electrons has to be taken zero everywhere except in the interior of a CQWR. It is supposed as well that only a charged channel contributes to the CQWR screening in presented model.

In the assumptions the externally applied charge  $-e$  produces a linear response in Q1D EG, for large enough distances when  $e\Phi_s \ll \mu_0$  we may expand  $\Delta n^{ind}(\rho, z)$  and obtain in leading order as

$$\Delta n_v(\rho, z) = \frac{\partial n^{ind}}{\partial \mu_0} e\Phi_s(\rho, z). \quad (2)$$

Together with the abovementioned assumptions a strong confinement condition would be assumed that the quantum wire radius is small compared with the Coulomb center Bohr radius  $a_0 = \epsilon_w \hbar^2 / m_e e^2$  for bulk samples ( $a_0 \gg R$ ). As follows, the distances along the wire axis  $|z| \gg R$  are essential in discussed case and therefore the long wave 1D region  $q \ll R^{-1}$  could be appropriate for the interaction screened potential in accordance with the TFA. This permits us to apply a geometrical adiabatic method introduced for the first time in Ref.[9] when discussing the Q2D EG properties of the QW system. Substituting equation (2) in the first equation of system (1) and expressing the screening potential  $V_s(\rho, z)$  in Fourier components as  $V_s(\rho, z) = \int_0^\infty V_s(\rho, q) e^{iqz} dq$  we will have

$$\left( \frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} \right) V_s(\rho, q) - \left[ q^2 + \frac{4\pi e^2}{\epsilon_w} \frac{\partial n^{ind}}{\partial \mu_0} \right] V_s(\rho, q) = -\frac{4\pi e^2}{\epsilon_w} \delta(\rho) \quad (3)$$

where  $q = k - k'$ . The latter is the linear equation with the variable coefficient in the middle term depending on the plane coordinate  $\rho$ . A characteristic spatial change of the quantity  $\partial n^{ind} / \partial \mu_0$  is significantly in the order of the CQWR radius  $R$ . As in Ref.[9] with the Q2D EG case, if replace the quantity  $\partial n^{ind} / \partial \mu_0$  in equation (3) by the latter's average value such as

$$\frac{\partial \bar{n}^{ind}}{\partial \mu_0} = \frac{1}{S} \int_0^R \frac{\partial n^{ind}}{\partial \mu_0} \rho d\rho d\varphi = \frac{1}{S} \frac{\partial \bar{n}_L}{\partial \mu_0}, \quad (4)$$

we can obtain linear equation

$$\left( \frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} \right) V_s - \tilde{q}^2 V_s = -\frac{4\pi e^2}{\varepsilon_w} \delta(\rho) \quad (5)$$

with the independent of the variable  $\rho$  coefficient  $\tilde{q}^2 = q^2 + q_s^2$ ,  $\bar{n}_L$  is the mean linear charge density,  $S = \pi R^2$  is the CQWR cross section area. Here in equation (5)

$$q_s = \sqrt{\frac{4\pi e^2}{\varepsilon_w} \frac{\partial \bar{n}_L}{\partial \mu_0}} \quad (6)$$

is the averaged TFA screening parameter.

As we can see from the Eq.(5) a characteristic spatial distance along the z axis in CQWR for that a solution of the equation changes appreciably, is order of the  $\tilde{q}^{-1}$ . If the condition  $\tilde{q}R \ll 1$  holds then, the sought potential  $V_s(\rho, q)$  from the Eq.(3) coincides with the solution of Eq.(5) and, hence, we must focus on the solution of the last equation. The most general solutions of the Eq.(5) both with the axial and reflection symmetry at the origin are [11, 12]

$$\begin{cases} V_s = \int_0^\infty \cos qz [A I_0(\tilde{q}\rho) + B K_0(\tilde{q}\rho)] dq, & \rho \leq R \\ V_s = \int_0^\infty \cos qz [C K_0(q\rho) + D I_0(q\rho)] dq, & \rho > R \end{cases}, \quad (7)$$

where  $I(x)$  and  $K(x)$  are modified Bessel functions. The coefficients  $A(q)$ ,  $B(q)$ ,  $C(q)$  and  $D(q)$  have been determined by applying the standard Maxwell boundary conditions at the CQWR surface and requiring the limiting asymptotic expressions of the electrostatic potential  $V_s(\rho, z)$  both at the origin and infinity. As a result, pair of the linear equations

$$\begin{cases} A I_0(\tilde{q}R) + \frac{2e}{\pi \varepsilon_w} K_0(\tilde{q}R) = C K_0(qR), \\ A \frac{\tilde{q}}{q \varepsilon_b} \varepsilon_w I_1(\tilde{q}R) - \frac{2e}{\pi q \varepsilon_b} \tilde{q} K_1(\tilde{q}R) = -C K_1(qR), \end{cases} \quad (8)$$

is derived, where the expressions  $D(q)=0$ ,  $B(q) = -2e^2/\pi \varepsilon_w$  are taken into account [12].

After combining solutions of Exps. (8) with the equation (7) for the sought 3D interaction screened potential of the semiconductor CQWR embedded in the dielectric barrier media obtain

$$\begin{cases} V_s = -\frac{2e^2}{\pi \varepsilon_w} \int_0^\infty dq \cos qz [K_0(\tilde{q}\rho) + I_0(\tilde{q}\rho)] \frac{[\varepsilon_r \tilde{q} K_0(qR) K_1(\tilde{q}R) - q K_0(\tilde{q}R) K_1(qR)]}{\varepsilon_r \tilde{q} K_0(qR) I_1(\tilde{q}R) + q K_1(qR) I_0(\tilde{q}R)}, \\ V_s = -\frac{2e^2}{\pi \varepsilon_b} \int_0^\infty dq \cos qz K_0(q\rho) \frac{\tilde{q} K_0(\tilde{q}R) I_1(\tilde{q}R) + \tilde{q} K_1(\tilde{q}R) I_0(\tilde{q}R)}{\varepsilon_r \tilde{q} K_0(qR) I_1(\tilde{q}R) + q K_1(qR) I_0(\tilde{q}R)}. \end{cases} \quad (9)$$

where  $\varepsilon_r = \varepsilon_w / \varepsilon_b$ . As follows, the screened potential in the QWR region consists of the homogeneous and inhomogeneous polarization connected parts such as:  $V_s = V_s^{\text{hom}} + V_s^{\text{inh}}$ . In the case of an infinite wire the potential inside the wire takes the fully screened 3D Debye-Hückel potential form as  $R \rightarrow \infty$

$$V_s(\rho, z) = -\frac{e^2}{\varepsilon_w} \frac{e^{-q_s \sqrt{\rho^2 + z^2}}}{\sqrt{\rho^2 + z^2}}. \quad (10)$$

For the case of infinitesimal wire or filament ( $R \rightarrow 0$ ) the screened potential outside the QWR takes the unscreened Coulomb potential form characterized by barrier dielectric constant

$$V(\rho, z) = -\frac{e^2}{\epsilon_b} \frac{1}{\sqrt{\rho^2 + z^2}}. \quad (11)$$

Note, that the equation (9) easily reduces to the appropriate unscreened CQWR 3D interaction potential forms (see Ref.[16]) if neglect the TFA screening parameter  $q_s$  in the effective Q1D wave vector expression  $\tilde{q} = \sqrt{q^2 + q_s^2}$ . In turn, the screened potential would be reduced as well to the metallic CQWR case expressions (Refs.[11, 12]) by substitution  $\epsilon_w = \epsilon_b = 1$ .

### 3. Dielectric confinement affected Q1D CQWR screening potential and effective screening radius

Now we will obtain CQWR Q1D interaction screened potential analytic expressions taking into account the DC effect. In order to get a general insight into the "Coulomb interaction engineering" possibilities of the DC effect a strong contrast between the dielectric constants  $\epsilon_w$  and  $\epsilon_b$  is accepted such as:  $\epsilon_r = \epsilon_w / \epsilon_b \gg 1$ .

In the previous section the condition  $\tilde{q}R \ll 1$  has been imposed meaning that the typical spatial change of the screened potential energy's Fourier-component is large enough than the CQWR radius. The latter will be realized when the following two conditions are simultaneously fulfilled

$$\begin{cases} qR \ll 1, \\ q_s R \ll 1. \end{cases} \quad (12)$$

With these conditions the screened potential takes the Q1D form such as

$$V_s^{Q1D}(z) = -\frac{e^2}{\epsilon_w} \frac{e^{-q_s|z|}}{|z|} - \frac{2e^2}{\pi\epsilon_w} \int_0^\infty \cos qz \frac{\epsilon_r \ln(qR)^{-1}}{\epsilon_r (\tilde{q}R)^2 \ln(qR)^{-1} + 1} dq. \quad (13)$$

If we neglect the DC effect, i.e. the condition  $\epsilon_r \sim 1$  would be imposed in equation (13), then 1D screened potential long wave limit result has to be restored (Exps.4.3-4.4 in Ref. [14]) in QWR.

As for the unscreened case in QWR [16, 18], for the asymptotic distances along the wire axis  $|z| \gg R$  there exists in equation (13) two distinct effective long wave vector ranges appropriate to the 1D moderate small and very small wave vectors. The latters are:  $\epsilon_r (qR)^2 \ln(qR)^{-1} \geq 1$  and  $\epsilon_r (qR)^2 \ln(qR)^{-1} \ll 1$ , respectively, for that the Q1D screened potential takes the following asymptotic analytic forms.

#### 3.1. A

For the intermediate distances  $|z| \gg R$  corresponding to the criteria

$$\epsilon_r \left(\frac{R}{z}\right)^2 \ln \frac{|z|}{R} \geq 1, \quad (14)$$

after identical transformations connected with the first wave vector inequality, the screened interaction potential takes the form

$$V_{Si}^{Q1D}(z) = -\frac{e^2}{\epsilon_w} \left[ \frac{e^{-q_s|z|}}{|z|} - \frac{2}{\pi R^2} \int_0^\infty \frac{\cos qz dq}{q^2 + \tilde{q}_s^2} \right]. \quad (15)$$

The latter, in turn, gives the result as

$$V_{Si}^{Q1D}(z) = -\frac{e^2}{\epsilon_w R} \left[ \frac{R}{|z|} e^{-q_s z} + \frac{1}{\tilde{q}_s R} e^{-\tilde{q}_s z} \right], \quad (16)$$

where

$$\tilde{q}_s = \frac{1}{R} \sqrt{\frac{2}{\varepsilon_r \ln \varepsilon_r} + q_s^2} . \quad (17)$$

From the standpoint of both long wave ( $q \ll R^{-1}$ ) and DC effect ( $\varepsilon_r = \varepsilon_w / \varepsilon_b \gg 1$ ) conditions, the main contribution in equation (16) connected with the inhomogeneous polarization related second term.

Afterwards, the screened interaction potential will take the final form

$$V_{si}^{Q1D}(z) = -\frac{e^2}{\varepsilon_w R} \frac{1}{\tilde{q}_s R} e^{-\tilde{q}_s z} . \quad (18)$$

As can be seen from equation (18) the DC affected screening potential deviates from the 3D and pure 1D screened potential forms. It takes the Q1D form and, as in the Q2D case [9], strongly enhances with the reducing of the QWR confinement length. The similar result is established in Ref.[14] as well, where the DC effect is out of the discussion.

Note, that the Q1D screening effect emerges for the moderately large  $|z| \gg R$  intercharge distances only, which is appropriate to the moderately thin quantum wires. The screened potential  $V_{si}^{Q1D}(z)$  strongly depends from the DC affected effective screening parameter  $\tilde{q}_s$  and, in turn, is enhanced due to the small parameter  $\tilde{q}_s R \ll 1$ . At the same time,  $V_{si}^{Q1D}(z)$  is exponentially weak enough outside of the spatial region with the linear size equal to  $z_s = \tilde{q}_s^{-1}$ , which is believed to be the effective Q1D screening distance in CQWR. Thereby takes place a recovering of the effective Q1D screening length, like a DC affected QW case [9, 25]. Besides that, the Q1D screening length  $z_s$  strongly depends on the dielectric constants ratio  $\varepsilon_r$ . As follows, accounting of the DC effect results that the screening effect becomes effective in this case.

Let now study the TFA screening averaged parameter after equation (6).

Within the framework of the TFA method it is believed that only one size-quantized energy subband is filled (the size quantum limit (SQL)) and that the spatial variation of the electrostatic potential is small over distances comparable to the mean electron de Broglie wavelength  $\lambda_{dB}$ . So in SQL the QWR is believed thin enough ( $R < \lambda_{dB}$ ) that the long wave condition  $qR < 1$  after equation (12) holds. In turn, the mean linear charge density  $\bar{n}_L$  after equation (6) is determined by 1D EG statistics at 0K as [24, 14]

$$n_L = \frac{4}{\pi \hbar} \sqrt{\frac{m_e}{2} E_F} , \quad (19)$$

where  $E_F = \hbar^2 k_F^2 / 2m_e$  is the Fermi energy of the 1D EG and the Fermi wave number is determined as  $k_F = \pi n_L / 2$ ,  $m_e$  is the electron effective mass. If combining the Exps. (6) and (19) we get

$$q_s = \frac{4}{\pi R} \left[ \frac{1}{a_0 n_L} \right]^{1/2} . \quad (20)$$

and

$$z_s = R \left[ \frac{2}{\varepsilon_r \ln \varepsilon_r} + \frac{16}{\pi^2 a_0 n_L} \right]^{-1/2} \quad (21)$$

The second inequality in (12) in accordance with equation (20) results that  $a_0 n_L \gg 1$ , i.e. the number of 1D electrons on the Bohr radius length should be large.

### 3.2. B

For the very large intercharge distances  $|z| \gg R$  corresponding to criteria

$$\varepsilon_r \left(\frac{R}{z}\right)^2 \ln \frac{|z|}{R} \ll 1 \quad (22)$$

and with the small enough related values of  $q_s$  such as  $\varepsilon_r (q_s R)^2 \ln(qR)^{-1} \ll 1$ , the screened potential with the second wave vector inequality goes to the form

$$V_{sii}^{Q1D}(z) = -\frac{e^2}{\varepsilon_b \sqrt{z^2 + R^2}}. \quad (23)$$

Equation (23) is appropriate to the extremely thin wires and illustrates the following features.

At first, the latter reduces to the 1D Coulomb screened potential when DC effect is absent (see equation (4.5) of Ref.[14]). In turn,  $V_{sii}^{Q1D}(z)$  is characterized, as in the unscreened case [16], by Q1D Coulomb law with the surrounding barrier environment small value dielectric constant. Thus, in the case of thin enough quantum wires, the Q1D screening effect is wholly suppressed regardless of the accounting the DC effect. That is fairly natural, since in the Q1D (1D) systems for the large enough intercharge distances  $z$ , the predominant part of the electric field lines extend outside the free carrier confinement region. As a result, the free carriers cannot effectively screen the Coulomb field between any two charges inside the thin enough quantum wire.

## 4. Conclusion

In summary, the asymptotic relatively simple expressions of the screened Coulomb interaction potential and effective screening length of the semiconductor CQWR embedded in the dielectric barrier media is derived. It is shown, that for the moderately thin DC influenced semiconductor CQWR the screened Q1D interaction potential to be

$$V_{si}^{Q1D}(z) = -\frac{e^2}{\varepsilon_w R \tilde{q}_s R} e^{-\tilde{q}_s z}. \quad (24)$$

The latter becomes strongly enhanced when reducing both wire radius and the Q1D effective screening parameter  $\tilde{q}_s$ . Expression of the DC affected effective Q1D screening length

$$z_s = \frac{R}{\left[ \frac{2}{\varepsilon_r \ln \varepsilon_r} + \frac{16}{\pi a_0 n_L} \right]^{1/2}} \quad (25)$$

is established in the TFA approximation, which strongly depends on the dielectric constants ratio  $\varepsilon_r$ . It is received, that, like a DC affected QW case, in DC influenced QWR system takes place a recovering of the effective Q1D screening length. It has been revealed as well that the screening effect does wholly diminish in thin enough quantum wire, in accordance with Q1D Coulomb law (23). The latter is characterized by barrier environment small dielectric constant as in the unscreened case.

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